

Surfactants as molecular switches in the formation of β structures in peptides.

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Surfactants, due to their amphiphilic structure, can simultaneously participate in electrostatic and hydrophobic interactions, influencing the properties of macromolecular systems. The importance of surfactants derives from their ability to change the conformation and aggregation of macromolecules, which translates into the functional properties of the systems. The interaction of sodium dodecyl sulfate (SDS), chosen as a model anionic surfactant, with short peptides containing 19-39 amino acids and its effect on the conformational structure was studied. A hybrid approach was used to capture the mechanisms responsible for the formation of β -structures. Peptide sequences were generated using an improved version of AIMS2.0 deep learning [1]. The stability of the structures and their self-assembly process were analyzed using molecular dynamics (MD) simulations in the GROMACS software. The simulations conducted allow for a detailed understanding of the molecular mechanisms. The obtained results indicate that SDS can induce a transition from a disordered form to stable β -hairpin structures in selected peptides, which has been confirmed experimentally. In addition, such transition results in better mechanical properties of the obtained materials. Collected observations suggest that surfactants can act as molecular switches, process controls, self-organization and formation of β structures. Our results bring new information on designing biomaterials with controlled mechanical properties.

References:

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